Contents of Volume 38

NUMBER 1 JANUARY 2000

Review Article

Isotope effects on chemical shifts of proteins and peptides
P. E. HANSEN 1

Solid-state NMR of bisphosphonates adsorbed on hydroxyapatite
G. GROSSMANN, A. GROSSMANN, G. OHMS, E. BREUER, R. CHEN, G. GOLOMB, H. COHEN, G. HÄGELE AND R. CLASSEN 11

Carbon-13 and mercury-199 nuclear spin relaxation study on solution dynamics of bis(phenylethynyl)mercury molecule and shielding anisotropy of its acetylenic carbon and mercury nuclei
A. GRYFF-KELLER AND S. MOLCHANOV 17

^{13}C NMR of Pd–aryl complexes. Chemical shifts and Pd π-back bonding
E. MARTINEZ-VIVIENTE, P. S. PREGOSIN AND M. TSCHOERNER 23

Chiral discrimination of methylphenylsulfoxide using dirhodium complexes
C. MEYER AND H. DUDDECK 29

Parahydrogen induced polarization in presence of NMR shift reagents
C. ULRICH AND J. BARGON 33

Notes

Complete analysis of the ^{31}P and ^{19}F NMR spectra of $[(PF_3)_3Mo(CO)_3]$
C. G. BARLOW, D. L. MILLER AND R. A. NEWMARK 38

^{1}H and ^{13}C NMR spectra of betaines, $>N^{+}(CH_2)_nCOO^{-}$, and their hydrogen halides. Additivity rules for carbon-13 chemical shifts
Z. DEGA-SZAFRAN, E. DULEWICZ AND M. SZAFRAN 43

Structural elucidation of two novel products from the soybean lipoxygenase-catalysed dioxygenation of curcumin
G. TÓTH, M. ROTH, B. WECKERLE AND P. SCHREIER 51

^{1}H and ^{13}C NMR study of 2-substituted phenyl methyl sulphides
S. PERUMAL, R. CHANDRASEKARAN, S. SELVARAJ, M. GANESAN AND D. A. WILSON 55

Rapid Communications

Doubling the sensitivity of natural abundance ^{13}C–^{13}C INADEQUATE with off-resonance compensation
J. BUNKENBORG, N. C. NIELSEN AND O. W. SØRENSEN 58

Rates of motion for free radicals in zeolites as directly measured by logitudinal field muon spin relaxation
C. J. RHODES, T. C. DINTINGER AND C. A. SCOTT 62

Papers in press, 66

NUMBER 2 FEBRUARY 2000

EPR and ENDOR on radicals of chlorin- and bacteriochlorin-quinone model compounds for electron transfer in photosynthesis
H. MÖßLER, M. WITTENBERG, D. NIETHAMMER, R. K. MUDRASSAGAM, H. KURRECK AND M. HUBER 67

Classical H-NMR shielding calculations with the program SHIFT and conformational analysis of three cyclophanes
V. RÜDIGER AND H.-J. SCHNEIDER 85

BF_4^- as a probe for ion pair solution structure using interionic one- and two-dimensional ^{19}F{^{1}H} NOEs
C. HOFSTETTER AND T. C. POCHAPSKY 90

Double-helical DNA ^{1}H chemical shifts: an accurate and balanced predictive empirical scheme
C. ALTONA, D. H. FABER AND A. J. A. WESTRA HOEKZEMA 95

Analysis of ^{1}H and ^{13}C NMR sectra of *cis*- and *trans*-10-substituted-decal-2-ones by 2D NMR techniques
G. DI MAIO, L. M. MIGNECO, E. VECCHI AND C. IAVARONE 108

Transmission of polar substituent effects across the bicyclo[1.1.1]pentane ring system as monitored by ^{19}F NMR shifts
W. ADCOCK AND A. R. KRSTIC 115

Notes
Conformational analysis of diribosylribitolphosphate by NMR and molecular dynamics
M. MAESTRE AND C. S. PÉREZ 123

On the ^{1}H chemical shift assignments for ampicillin
J. C. TUNG, A. J. GONZALES, J. D. SADOWSKY AND D. J. O'LEARY 126

Complete assignment of ^{1}H and ^{13}C NMR spectra of a set of sulphinyl and sulphonyl monomers toward poly(*p*-phenylene vinylene) precursors
A. J. J. M. VAN BREEMEN, A. C. J. ISSARIS, M. M. DE KOK, P. J. ADRIAENSENS, D. J. M. VANDERZANDE AND J. M. J. V. GELAN 129

Complete assignment of the ^{13}C NMR spectra of 4,4-dimethylanthracene-1,9,10(4*H*)-trione and the regioisomeric monomethyl derivatives
R. ARAYA-MATURANA, W. CARDONA, T. DELGADO-CASTRO AND C. JULLIAN 135

Reference Data
^{1}H and ^{13}C NMR spectral assignments of some tetracyclic phenothiazine derivatives
F. CHATEL, R. FAURE, G. BOYER AND J. P. GALY 137

^{1}H and ^{13}C NMR spectral assignment of phytochelatin
E. YOSHIMURA, R. KOBAYASHI, K. FURIHATA, H. KAJIWARA AND S. YAMAZAKI 141

Rapid communication
Constant time inverse-detection gradient accordion rescaled heteronuclear multiple bond correlation spectroscopy: CIGAR-HBMC
C. E. HADDEN, G. E. MARTIN AND V. V. KRISHNAMURTHY 143

Papers in press, 148

NUMBER 3 MARCH 2000

Giao NMR calculations for carbazole, and its *N*-methyl and *N*-ethyl derivatives. Comparison of theoretical and experimental ^{13}C chemical shifts
T. KUPKA, G. PASTERNA, M. JAWORSKA, A. KARALI AND P. DAIS 149

Application of frequency domain deconvolution to DQF–COSY spectra for the determination of coupling constants as a tool for signal assignment based on coupling networks
D. JEANNERAT 156

Dynamic NMR study of tri-*tert*-butylcarbinol and of a carbinol–methylaluminoxane mixture
T. HELAJA, K. HAKALA, J. HELAJA, B. LÖFGREN AND T. HASE 165

Push–pull and pull–push effects in isatylidenes
M. S. MORALES-RÍOS, M. GARCÍA-VELGARA, H. CERVANTES-CUEVAS, C. ALVAREZ-CISNEROS AND P. JOSEPH-NATHAN 172

Study of hydrogen bonding and solvent polarity effects on the nitrogen NMR shieldings of *N*,*N*-dimethylacetamidine
M. WITANOWSKI, W. SICINSKA, Z. BIEDRZYCKA AND G. A. WEBB 177

ESR spin-trap study of the radicals present during the thermolysis of some bis(*tert*-alkylperoxy)-alkanes and bis(*tert*-alkylperoxy)cycloalkanes
P. G. MEKARBANE AND B. J. TABNER 183

Notes

Thermodynamical stability of indazole studied by NMR–NQR spectroscopy and *ab initio* calculations
J. N. LATOSIŃSKA 192

Hydrogen bonding in diethyl 2-hydroxypropylphosphonate—an example of equilibrium between intramolecular and intermolecular bonding
R. GANCARZ, R. LATAJKA, B. MAŁUSZEK, E. ŻYMAŃCZYK-DUDA AND P. KAFARSKI 197

Complete assignment of the ^{1}H and ^{13}C NMR spectra of four triterpenes of the ursane, artane, lupane and friedelane groups
J. S. ALVES, J. C. M. DE CASTRO, M. O. FREIRE, E. V. L. DA-CUNHA, J. M. BARBOSA-FILHO AND M. S. DA SILVA 201

Reference Data

Benzodiazepine analogues. Part 19. ^{1}H and ^{13}C NMR spectroscopic studies of 2-phenyl-1,4- and 1,5-benzoheterazepinethione derivatives
M. J. MPHAHLELE AND P. T. KAYE 207

^{1}H and ^{13}C NMR spectroscopy of 6-aryl-substituted 3-[5-methyl-1-(4-methylphenyl)-1,2,3-triazol-4-yl]-*s*-triazolo[3,4-b]-1,3,4-thiadiazoles
H.-S. DONG, B. QUAN, K. WEI, Q.-L. WANG AND Z.-Y. ZHANG 210

Substituent effects on ^{13}C and ^{1}H chemical shifts in 2-isopropyl- and 2,6-biisopropylnaphthalene and their oxidation products
R. MAZURKIEWICZ AND J. ZAWADIAK 213

Rapid Communication

Examination of subsequent reaction products enhanced through parahydrogen-induced nuclear polarization (PHIP)
A. KOCH AND J. BARGON 216

Papers in press, 221

NUMBER 4 APRIL 2000

Unidentate coordination of 2,2′-bipyridine and 1,10-phenanthroline in a cyclometallated rhodium(III) complex. Evidence from ^{1}H and ^{13}C NMR spectra
G. A. NAGANAGOWDA, K. V. RAMANATHAN, V. GAYATHRI AND N. M. NANJE GOWDA 223

3D structure of microperoxidase-11 by NMR and molecular dynamic studies
R. MONDELLI, L. SCAGLIONI, S. MAZZINI, G. BOLIS AND G. RANGHINO 229

^{13}C NMR chemical shift as a probe for estimating the conformation of aromatic groups in the solid state. 1. Biphenyls
S. ANDO, T. HIRONAKA, H. KUROSU AND I. ANDO 241

Application of accordion excitation in ^{1}H–^{15}N long-range heteronuclear shift correlation experiments at natural abundance
G. E. MARTIN AND C. E. HADDEN 251

N-1 and N-2 positional effects in the propagation of 3_{10}-type fold in the helical model peptide Boc-(D)Glu-Pro-Ala-Lys-Ala-Leu-Ala-OMe
S. BERI, S. SRIVASTAVA, M. DHANASEKARAN, R. S. PHADKE AND S. DURANI 257

One- and two-dimensional gradient-selected HSQMBC NMR experiments for the efficient analysis of long-range heteronuclear coupling constants
R. T. WILLIAMSON, B. L. MÁRQUEZ, W. H. GERWICK AND K. E. KÖVÉR 265

NMR structure determination of brefeldin-A, a 13-membered ring fungal metabolite
R. GLASER, D. SHIFTAN AND M. FROIMOWITZ 274

Mobility of dichloroethyl radicals sorbed in kaolin and silica: a potential model of heterogeneous atmospheric processes
C. J. RHODES, T. C. DINTINGER, I. D. REID AND C. A. SCOTT 281

^{31}P–^{1}H correlation and resonance assignments along the DNA backbone: three-dimensional implementation of heteronuclear long-range correlation experiment
V. K. RASTOGI 288

^{15}N, ^{13}C and ^{1}H NMR study of azo coupling products from diazonium salts and enaminones
V. MACHÁČEK, A. LYČKA, P. ŠIMŮNEK AND T. WEIDLICH 293

Notes
Structure determination by ^{1}H and ^{13}C NMR of a new flavan isolated from *Brosimum actifolium*: 4′,7-dihydroxy-8-prenylflavan
A. F. TEIXEIRA, A. F. C. ALCANTARA AND D. PILO-VELOSO 301

Combined variable temperature and variable field ^{15}N cross-polarization magic angle spinning NMR study of ^{15}N, ^{14}N residual dipolar coupling in pyrazole derivatives
S. H. ALARCÓN, J. A. JIMÉNEZ, R. M. CLARAMUNT, H.-H. LIMBACH AND J. ELGUERO 305

Heteronuclear editing method for detecting NOE between chemically equivalent protons: application to polycyclic aromatic hydrocarbons
R. E. HOFFMAN, R. SHENHAR, I. WILLNER, H. E. BRONSTEIN, L. T. SCOTT, A. RAJCA AND M. RABINOVITZ 311

Rapid Communication
Improving bioaffinity NMR spectra by means of zero-quantum dephasing
T. WEIMAR 315

Conference report, 319; Papers in press, 320

NUMBER 5 MAY 2000

Direct measurement of heteronuclear long-range coupling constants from phase-sensitive HMBC spectra
K. DING 321

NMR studies of calcium-induced alginate gelation. Part 1—MRI tests of gelation models
J.-M. DUEZ, M. MESTDAGH, R. DEMEURE, J.-F. GOUDEMANT, B. P. HILLS AND J. GODWARD 324

Separation of cross-relaxation and chemical exchange effects in magnetization transfer experiments: application to a trialkylaluminium–dialkylamine complex
E. S. BENTO, D. C. BRADLEY, G. E. HAWKES, I. A. MAIA AND K. D. SALES 331

Application of immobilized free radicals in supercritical fluid chromatography hyphenated with proton nuclear magnetic resonance spectroscopy
H. FISCHER, L.-H. TSENG, M. RAITZA AND K. ALBERT 336

Effect of oxygen substituents on two- and three-bond carbon–proton spin–spin coupling constants
M. MORVAI, T. NAGY, A. KOCSIS, L. F. SZABÓ AND B. PODÁNYI 343

Notes
Stereochemical assignment of the meridional isomer of the trisbidentate chelate complex $Ga(fox)_3$ (fox = 5-fluoro-8-hydroxyquinoline) by two-dimensional correlated NMR
O. JARJAYES, S. HAMMAN, M.-C. BROCHIER, C. BÉGUIN AND R. NARDIN 360

Total assignment of the ^{1}H and ^{13}C NMR spectra of casimiroedine and its peracetylated derivative
W. F. REYNOLDS, R. G. ENRIQUEZ, G. A. MAGOS AND D. GNECCO 366

^{1}H NMR studies of rotational isomerism in phosphonic analogues of aspartic acid
D. JĘDRZEJCZYK, Z. ZIORA AND PANEE KAFARSKI 370

Reference Data
^{1}H and ^{13}C NMR spectroscopy of brominated diphenyl ethers. A multiple linear regression analysis
J. HU, E. KOLEHMAINEN AND J. KNUUTINEN 375

A ^{1}H, ^{13}C, ^{31}P and ^{15}N NMR study of (pyrrolidine-2,2-diyl)bisphosphonic acid, tetraalkyl-(pyrrolidine-2,2-diyl)bisphosphonates and acyclic tetraethyl bisphosphonates
G. OLIVE AND M. H. P. VAN GENDEREN 379

^{1}H and ^{13}C NMR chemical shift assignment of some *N*-bromoalkyl-(*E*)-4-azachalcone bromides
Z. NOWAKOWSKA 382

α-Phenylsulfonyl-*N*-arylacetamides (α-phenylsulfonylacetanilides): ^{1}H, ^{13}C and ^{15}N NMR spectral characterization
E. KOLEHMAINEN, H. JANOTA, R. GAWINECKI, K. LAIHIA AND R. KAUPPINEN 384

^{13}C NMR spectral characterization of *N*-aryl-substituted 4*H*-1,4-benzothiazine 1,1-dioxide derivatives
S. E. LÓPEZ, M. V. GODOY, J. CHARRIS, N. URDANETA, J. SALAZAR AND A. I. PUIG 386

Atom connectivity and spectral assignments from the ^{29}Si–^{29}Si INADEQUATE experiment on a nanometer scale dendritic polysilane
J. B. LAMBERT AND H. WU 388

^{13}C NMR substituent chemical shifts in hydroxy-*p*-benzoquinones
E. BURGUEÑO-TAPIA AND P. JOSEPH-NATHAN 390

NUMBER 6 JUNE 2000

A DFT/GIAO/NBO and experimental study of ^{13}C SCSs in 1-X-bicyclo[1.1.1]pentanes
E. W. DELLA, I. J. LOCHERT, J. E. PERALTA AND R. H. CONTRERAS 395

Comparative ^{13}C and ^{2}H relaxation study of microsecond dynamics of the AT tract of selectively ^{13}C/^{2}H double-labelled DNA duplexes
T. V. MALTSEVA, A. FÖLDESI, D. OSSIPOV AND J. CHATTOPADHYAYA 403

High resolution in the indirectly detected dimension exploiting the processing of folded spectra
D. JEANNERAT 415

Effects of temperature on the ESR and ENDOR spectra of the DMPO–OBu^{t} spin adduct; the problems of identifying the trapped radical
J. D. HONEYWILL AND B. MILE 423

NMR quantification in hydrothermal *in situ* syntheses
C. GERARDIN, M. HAOUAS, C. LORENTZ AND F. TAULELLE 429

^{1}H NMR as a tool for the analysis of mixtures of virgin olive oil with oils of different botanical origin
C. FAUHL, F. RENIERO AND C. GUILLOU 436

Towards the automatic analysis of ^{1}H NMR spectra
L. GRIFFITHS 444

The accordion-HMQC: heteronuclear correlations for a range of coupling constants
K. ZANGGER AND I. M. ARMITAGE 452

Application of adiabatic inversion pulses for elimination of baseline distortions in Fourier transform NMR. A natural abundance ^{17}O NMR spectrum for gaseous acetone
W. KOŹMIŃSKI AND K. JACKOWSKI 459

Notes
Synthesis, NMR and molecular modeling studies on the stereochemistry of 2-aryl-3-(2′,4′-dinitrophenylthio)cyclohexenes
V. C. DEVANATHAN, S. PERUMAL, M. J. E. HEWLINS AND M. RAMALINGAM 463

Downfield chemical shifts at α-protons and carbons of β-propiothiolactones
H. B. LEE, H.-Y. PARK, B.-S. LEE AND Y. G. KIM 468

Reference Data
NMR spectral data of salazinic acid isolated from some species of *Parmotrema*
V. L. EIFLER-LIMA, A. SPERRY, S. SINBANDHIT, J. BOUSTIE, S. TOMASI AND E. SCHENKEL 472

^{1}H and ^{13}C NMR spectra of commercial rhodamine ester derivatives
S. S. RAMOS, A. F. VILHENA, L. SANTOS AND P. ALMEIDA 475

^{1}H and ^{13}C NMR spectroscopic analysis of a series of unsaturated hexenones and heptenones
D. C. BYRD, K. W. STEWART AND J. B. GRUTZNER 479

^{1}H, ^{13}C and ^{15}N NMR and GIAO CPHF calculations on two quinoacridinium salts
J. JAROSZEWSKA-MANAJ, D. MACIEJEWSKA AND I. WAWER 482

NUMBER 7 JULY 2000

This Issue is Dedicated to Professor Dr Harald Günther on the Occasion of his 65th Birthday

Guest Editor: R. K. Harris

Editorial
R. K. HARRIS 487

Assignment of ^{1}H and ^{13}C spectra and investigation of hindered side-chain rotation in lupeol derivatives
D. BURNS, W. F. REYNOLDS, G. BUCHANAN, P. B. REESE AND R. G. ENRIQUEZ 488

^{1}H and ^{13}C NMR study of copteroside E derivatives
C. M. CERDA-GARCÍA-ROJAS, G. ZAMORANO, M. I. CHÁVEZ, C. A. N. CATALÁN AND P. JOSEPH-NATHAN 494

Application of DPFGSE-ROE to calixarene derivatives under conditions near NOE zero-crossing
W. BAUER, A. SOI AND A. HIRSCH 500

NMR studies of exchange between triazine rotamers
H. E. BIRKETT, R. K. HARRIS, P. HODGKINSON, K. CARR, M. H. CHARLTON, J. C. CHERRYMAN, A. M. CHIPPENDALE AND R. P. GLOVER 504

^{17}O NMR spectroscopy of 1-(2-hydroxyphenyl)-3-naphthylpropane-1,3-diones. Influences of keto–enol tautomerism and substituents
J. L. JIOS AND H. DUDDECK 512

Dynamic NMR study at a 1,3-diyne bridged dinuclear bis(cyclopentadienyl)titanium complex: understanding the C—C single bond metathesis reaction
W. BAUMANN, P.-M. PELLNY AND U. ROSENTHAL 515

Isotope-induced chemical shifts $^{1}\Delta^{12/13}C(^{29}Si)$ and ^{57}Fe NMR of organosubstituted 2,5-dihydro-1,2,5-azasilaboroles, a silole and their tricarbonyliron complexes
B. WRACKMEYER, G. SEIDEL AND R. KÖSTER 520

Primary tritium and deuterium isotope effects on chemical shifts of compounds having an intramolecular hydrogen bond
S. BOLVIG, P. E. HANSEN, H. MORIMOTO, D. WEMMER AND P. WILLIAMS 525

Mapping the effects of metal ion reduction and substrate analog binding to Fe-superoxide dismutase by NMR spectroscopy
S. VATHYAM, R. A. BYRD AND A.-F. MILLER 536

^{1}H NMRD profiles of diamagnetic proteins: a model-free analysis
I. BERTINI, M. FRAGAI, C. LUCHINAT AND G. PARIGI 543

Fluorine as an NMR probe for structural studies of chemical and biological systems
Y. G. GAKH, A. A. GAKH AND A. M. GRONENBORN 551

Investigation of ^{19}F–^{19}F spin–spin coupling in 1-(x-fluorophenyl)-8-(y-fluorophenyl)naphthalenes (x, y = 2, 3, 4)
L. ERNST AND P. SAKHAII 559

Experimental and quantum chemical investigation of the stereochemical dependence of spin coupling constants in symmetrical strained alkenes
S. BERGER, A. KREBS, B. THÖLKE AND H.-U. SIEHL 566

Proton chemical shifts in NMR. Part 15—Proton chemical shifts in nitriles and the electric field and π-electron effects of the cyano group
R. J. ABRAHAM AND M. REID 570

Solvent effects on the nitrogen NMR shieldings of 3-methylsydnone and *ab initio* calculations of the shieldings including related oxazole and oxadiazole systems
M. WITANOWSKI, Z. BIEDRZYCKA AND Z. GRABOWSKI 580

High-resolution ^{1}H NMR spectroscopy of absorbed molecules in the presence of strong magnetic fields
J. ROLAND AND D. MICHEL 587

Solid-state NMR study of the SH3 domain of α-spectrin: application of ^{13}C–^{15}N TEDOR and REDOR
S. MACHOLL, I. SACK, H.-H. LIMBACH, J. PAULI, M. KELLY AND G. BUNTKOWSKY 596

Triple proton transfer in crystalline 3,5-dibromo-1*H*-1,2,4-triazole and 3,5-dichloro-1*H*-1,2,4-triazole studied by variable-temperature ^{15}N NMR and *ab initio* calculations
M. A. GARCÍA, C. LÓPEZ, O. PETERS, R. M. CLARAMUNT, O. KLEIN, D. SCHAGEN, H.-H. LIMBACH, C. FOCES-FOCES AND J. ELGUERO 604

Papers in press, 615

NUMBER 8 AUGUST 2000

Nitrogen NMR study of some mesoionic oxadiazoles and thiadiazoles
J. JAŹWIŃSKI, O. STASZEWSKA, J. W. WIENCH, L. STEFANIAK, S. ARAKI AND G. A. WEBB 617

Axial/equatorial populations in α-hetero-substituted cyclohexanone oximes and *O*-methyl oximes
D. S. RIBEIRO, P. R. OLIVATO AND R. RITTNER 627

Structure of *p*-tetrafluorobenzoquinone: interaction with nematic liquid crystals
Y. ARFAOUI AND E. HALOUI 639

Radiolabelling studies of free radical reactions using muonium (the second hydrogen radioisotope): evidence of a direct antioxidant role for vitamin k in repair of oxidative damage to lipids
C. J. RHODES, T. C. DINTINGER, H. A. MOYNIHAN AND I. D. REID 646

^{14}N-NMR spectroscopy of tertiary amines in supercritical fluids
S. GAEMERS AND C. J. ELSEVIER 650

Dynamic NMR study of rotational isomerism in the carbanion of *p*-trifluoromethanesulfonylbenzyltriflone in aprotic solvents
M. GROMOVA, C. G. BÉGUIN, R. GOUMONT, N. FAUCHER, M. TORDEUX AND F. TERRIER 655

High pressure ^{1}H NMR on model biomembranes: a study of the local anaesthetic tetracaine incorporated into POPC lipid bilayers
J. EISENBLÄTTER, A. ZENERINO AND R. WINTER 662

^{31}P NMR INEPT spectroscopy: a powerful tool for structural analysis of phosphitylated carbohydrates
L. POUYSÉGU, B. DE JÉSO, J. C. LARTIGUE, M. PÉTRAUD AND M. RATIER 668

Complete ^{1}H and ^{13}C NMR signal assignments of glaucolide B
A. V. COSTA, L. C. DE ALMEIDA BARBOSA, J. L. C. LOPES AND D. PILÓ-VELOSO 675

Notes
^{1}H and ^{13}C NMR study of the antihypertensive drugs nifedipine, nicardipine and related compounds
M. S. MORALES-RÍOS, A. DE LA CERDA MEDINA, V. PÉREZ-ALVAREZ AND P. JOSEPH-NATHAN 680

Flavone glycosides containing acetylated sugars from *Sideritis hyssopifolia*
Mª. L. RODRÍGUEZ-LYON, A. M. DÍAZ-LANZA, M. BERNABÉ AND L. VILLAESCUSA-CASTILLO 684

A new phenylpropanoid glycoside isolated from *Scrophularia scorodonia* L.
J. DE SANTOS GALÍNDEZ, A. M. DÍAZ-LANZA, L. F. MATELLANO AND A. R. SÁNCHEZ 688

Rapid Communications
New methods for measuring ^{1}H–^{31}P coupling constants in nucleic acids
C. H. GOTFREDSEN, A. MEISSNER, J. Ø. DUUS AND O. W. SØRENSEN 692

Reference Data

NMR spectral data for ester prodrugs of ganciclovir
H. GAO AND A. K. MITRA 696

^{1}H and ^{13}C NMR of acetyl derivatives of shamimin, a flavonol-*C*-glycoside
S. FAIZI AND M. ALI 701

NMR studies on synthesized diosgenyl saponin analogs
H. YU, X. W. HAN, X. M. LIU, B. YU, Y. Z. HUI AND X. BAO 704

NUMBER 9 SEPTEMBER 2000

An NMR study of the Lythraceae alkaloids
D. W. HUGHES, I. D. SPENSER AND J. T. WROBEL 707

NMR studies of calcium induced alginate gelation. Part II. The internal bead structure
B. P. HILLS, J. GODWARD, M. DEBATTY, L. BARRAS, C. P. SATURIO AND C. OUWERX 719

Sorption of benzene in caption-exchanged zeolite X, as measured by longitudinal field muon spin relaxation (LF-MuSRx)
C. J. RHODES, T. C. DINTIGER AND C. A. SCOTT 729

NMR structural study of cycloadducts obtained by hetero-Diels–Alder reaction of chiral 1-oxa-1,3-butadienes
H. DVOŘÁKOVÁ, R. HRABAL AND L. KNIEŽO 738

***In situ* PHIP-NMR studies during the stereoselective hydrogenation of sorbic acid with a $[Cp^{*}Ru]^{+}$ catalyst**
H. G. NIESSEN, D. SCHLEYER, S. WIEMANN, J. BARGON, S. STEINES AND B. DRIESSEN-HOELSCHER 747

NMR analysis of the configuration and conformation of *N*-acetylneuraminosyl-(2→3)-lactose
J. SCHULTE, J. LAUTERWEIN AND U. HÖWELER 751

Solution conformation of alkaloid chelidonine and its protonated form
P. KRAJEWSKI, L. KOZERSKI, G. GRYNKIEWICZ, E. BEDNAREK AND J. SITKOWSKI 757

Anomalous proton NMR relaxation behavior of cell wall materials from Chinese water chestnuts
H.-R. TANG, B.-L. ZHAO, P. S. BELTON, L. H. SUTCLIFFE AND A. NG 765

Room-temperature (^{1}H, ^{13}C) and variable-temperature (^{1}H) NMR studies on spinosin
K. C. LEWIS, A. R. MAXWELL, S. MCLEAN, W. F. REYNOLDS AND R. G. ENRIQUEZ 771

Photochromic spin traps. Part IV. 3,3-Diphenyl-5-[2-(*N-tert*-butylethanalnitrone)]-[3*H*]-naphtho-[2,1-*b*]pyran
A. ALBERTI, M. CAMPREDON, G. GIUSTI, B. LUCCIONI-HOUZE AND D. MACCIANTELLI 775

Improved high-resolution diffusion filtered ^{1}H MAS NMR
J. CHIN, A. CHEN AND M. J. SHAPIRO 782

Isofenchylic alcohol derived from a functionalized pinene oxide: unexpected formation and structural confirmation using multidimensional NMR spectroscopy and x-ray crystallography
M. VIALEMARINGE, M. J. BOURGEOIS, E. MONTAUDON, C. COURSEILLE, B. BARBE AND I. PIANET 785

Novel relaxation compensated method to measure proton exchange rates in biomolecules based on decorrelation of heteronuclear two-spin order
V. V. KRISHNAN AND M. COSMAN 789

Structure determination of dihydroxamic acids and their trimethylsilyl derivatives by NMR spectroscopy
J. SCHRAML, M. KVÍČALOVÁ, V. BLECHTA, L. SOUKUPOVÁ, O. EXNER, H.-M. BOLDHAUS, F. ERDT AND C. BLIEFERT 795

Notes

Complete assignments of ^{1}H and ^{13}C NMR spectra of four hispanane diterpenoids
B. RODRÍGUEZ AND G. SAVONA 802

Complete ^{1}H and ^{13}C chemical shift assignments of the new C_{22}-quassinoid isolated from *Picrolemma sprucei* Hook by NMR spectroscopy
I. J. C. VIERA, E. RODRIGUES-FILHO, J. B. FERNANDES, M. F. G. F. DA SILVA AND P. C. VIEIRA 805

Total assignment of ^{1}H and ^{13}C NMR spectra of two isomeric cucurbitane triterpenoids
F. J. Q. MONTE, S. M. A. PAPA, J. P. KINTZINGER AND R. BRAZ-FILHO 809

NUMBER 10 OCTOBER 2000

$^{37,35}Cl$ isotope effects on ^{19}F and ^{13}C chemical shifts of chlorofluoro- and hydrochlorofluorocarbons
A. FORIS 813

NMR study of intramolecular chemical exchange in the La(III) complex of triethylenetetraamine-hexaacetic acid in aqueous solution
S.-G. LEE 820

Evidence for the solvation of hydrogen atoms by water
M. C. R. SYMONS, C. J. RHODES AND I. D. REID 823

Multiple selective excitation as a tool for NMR studies of paramagnetic metalloproteins
N. GOASDOUE, D. RIVIERE, I. CORREIA, O. CONVERT AND M. PICCIOLI 827

OH–D_2 (OD–H_2) isotopic exchange at the surface of CaO monitored by electron paramagnetic resonance
P. PESCARMONA, M. CHIESA, M. C. PAGANINI AND E. GIAMELLO 833

Application of HECADE method to the measurement of long-range heteronuclear ^{13}C, ^{1}H spin–spin coupling constants in tautomeric β-sulfonylenamines
W. KOŹMIŃSKI, E. BEDNAREK, W. BOCIAN, J. SITKOWSKI, P. E. HANSEN, B. KWIECIEŃ AND L. KOZERSKI 839

ESR spin-trap study of the radicals present during the thermolysis of some novel alkyl peroxy esters
P. G. MEKARBANE AND B. J. TABNER 845

^{7}Li solid-state NMR spectroscopic study of aryllithium complexes: effects of aggregation and solvation
A. BOMAN AND D. JOHNELS 853

NMR spectroscopic and computational study of static and dynamic *E/Z* isomerism in aminoiminophosphines $R_2N—P{=}NMes^*$
D. GUDAT, W. HOFFBAUER, A. B. ROZHENKO, W. W. SCHOELLER AND M. I. POVOLOTSKII 861

Slow inversion of stereoisomers of cyclic GABA analogues
R. GANCARZ, R. LATAJKA, A. HALAMA AND P. KAFARSKI 867

Notes

NMR spectroscopy in partially oriented phases. Routine ^{2}H NMR of small to medium sized molecules
G. SZALONTAI 872

3α,3′α-Bis(*n*-acetoxyphenylcarboxy)-5β-cholan-24-oic acid ethane-1,2-diol diesters ($n = 2$–4): ^{13}C NMR chemical shifts, variable-temperature and NOE ^{1}H NMR measurements and MO calculations of novel bile acid-based dimers
J. TAMMINEN, E. KOLEHMAINEN, J. LINNANTO, H. SALO AND P. MÄNTTÄRI 877

NMR study of the stereochemistry of 2,4,6, 8-tetraaryl-3,7-diazabicyclo[3.3.1]nonan-9-ones
V. VIJAYAKUMAR, M. SUNDARAVADIVELU, S. PERUMAL AND M. J. E. HEWLINS 883

Concentration dependence of ^{13}C NMR spectra of triglycerides: implications for the NMR analysis of olive oils
L. MANNINA, C. LUCHINAT, M. PATUMI, M. C. EMANUELE, E. ROSSI AND A. SEGRE 886

Reference Data

^{13}C NMR chemical shift assignments for substituted 2-azabicyclo[3.3.1]nonan-3-ones
J. QUIRANTE, C. ESCOLANO, F. DIABA, M. TORRA AND J. BONJOCH 891

Analysis of the NMR spectra of some dimethylsilanes
A. D. BAIN, M. A. BROOK, P. HAZENDONK, D. REID AND R. S. STAN 894

NUMBER 11 NOVEMBER 2000

Studies on the solution-phase ESR spectra of the C_{60} monoanion under varying experimental conditions
R. D. WEBSTER 897

Determination of the substitution pattern of di- and trisubstituted pyrazines by ^{15}N, ^{13}C and ^{1}H NMR spectroscopy
H. SOMMER, H.-J. BERTRAM, G. E. KRAMMER, C. O. SCHMIDT, W. STUMPE, P. WERKHOFF AND M. ZVIELY 907

Oxygen-17 and deuterium NMR investigation into the adsorption of water on activated carbon
L. M. DICKINSON, R. K. HARRIS, J. A. SHAW, M. CHINN AND P. R. NORMAN 918

NMR study of 9-(1-adamantylaminomethyl)-9,10-dihydroanthracene and its β-cyclodextrin complexes
M. SÁNCHEZ, T. PARELLA, E. CERVELLÓ, C. JAIME AND A. VIRGILI 925

Correlated rotation in a conformationally restricted amide
E. R. JOHNSTON, R. FORTT AND J. C. BARBORAK 932

Structural characterization by NMR of rifabutinol, a derivative of rifabutin
L. SANTOS, F. FANT, M. A. MEDEIROS, F. A. M. BORREMANS, M. C. COSTA AND M. J. M. CURTO 937

Changes in *lac* Operator dynamics upon selective interaction with *lac* Repressor as revealed by heteronuclear relaxation rate measurements
F. PAQUET, J.-C. MAURIZOT AND G. LANCELOT 946

Identification of trifluoperazine metabolites using HPLC–NMR of test mixtures
M. DACHTLER, H. HÄNDEL, T. GLASER, D. LINDQUIST, R. M. HAWK, C. N. KARSON, R. A. KOMOROSKI AND K. ALBERT 951

Thermally initiated radical reactions of $K_2S_2O_8$: EPR spin trapping investigations
A. STAŠKO, V. BREZOVÁ, M. LIPTÁKOVÁ AND J. ŠAVEL 957

BIRD–HMBC: improved detection of heteronuclear long-range couplings
R. BURGER, C. SCHORN AND P. BIGLER 963

Notes

Predicting the Claisen rearrangement regioselectivity of allylindanyl and allyltetrahydronaphthalenyl ether derivatives by ^{1}H NMR experiments
D. C. RODRIGUES, S. A. FERNANDES AND A. J. MARSAIOLI 970

Ditetradecyl selenide, $(C_{14}H_{29})_2Se$, a new chemical shift reference compound for ^{77}Se NMR
K. I. DOUDIN, N. Å. FRØYSTEIN AND J. SONGSTAD 975

Two epimeric friedelane triterpenes isolated from *Maytenus truncata* Reiss: ^{1}H and ^{13}C chemical shift assignments
G. C. M. SALAZAR, G. D. F. SILVA, L. P. DUARTE, S. A. VIEIRA FILHO AND I. S. LULA 977

Rapid Communication
Economizing spectrometer time and broadband excitation in small-molecule heteronuclear NMR correlation spectroscopy. Broadband HMBC
A. MEISSNER AND O. W. SØRENSEN 981

Book reviews, 985: Papers in press, 986

NUMBER 12 DECEMBER 2000

***Ab initio* study of halogenated diphenyl ethers. NMR chemical shift prediction**
J. ELORANTA, J. HU, R. SUONTAMO, E. KOLEHMAINEN AND J. KNUUTINEN 987

Configurational and conformational analysis of *O*-vinyl ketoximes by ^{1}H and ^{13}C NMR spectroscopy
A. V. AFONIN, I. A. USHAKOV, S. V. ZINCHENKO, O. A. TARASOVA AND B. A. TROFIMOV 994

^{17}O NMR spectra of some Meisenheimer adducts
V. MACHÁČEK, A. LYČKA AND J. KAVÁLEK 1001

NMR analysis of tri- and tetrasaccharides from asparagus
E. FUKUSHI, S. ONODERA, A. YAMAMORI, N. SHIOMI AND J. KAWABATA 1005

Multiple-field carbon-13 and proton relaxation in sucrose in viscous solution
M. EFFEMEY, J. LANG AND J. KOWALEWSKI 1012

^{1}H and ^{13}C NMR assignments and conformational analysis of some podocarpene derivatives
M. ARNÓ, M. A. GONZÁLEZ, M. L. MARIN AND R. J. ZARAGOZÁ 1019

Notes
Complete assignment of the ^{1}H and ^{13}C NMR spectra of a new polyester sesquiterpene from *Austroplenckia populnea*
S. A. VIEIRA FILHO, L. P. DUARTE, M. H. SANTOS, G. D. F. SILVA, I. S. LULA AND R. J. C. F. AFONSO 1023

Total assignment of ^{1}H and ^{13}C NMR spectra of a prenylated oxanthrone from *Vismia latifolia*
M. H. DOS SANTOS, T. J. NAGEM, L. G. FONSECA E SILVA AND M. C. DA SILVA 1027

^{1}H and ^{13}C NMR assignments for the 3-deoxyanthocyanins, luteolinidin-5-glucoside and apigeninidin-5-glucoside
E. E. SWINNY, S. J. BLOOR AND H. WONG 1031

Reference Data
Experimental and calculated ^{13}C chemical shifts for α-, β-, γ-, and δ-carbolines
R. P. CORBALLY, L. K. MEHTA, J. PARRICK AND E. L. SHORT 1034

^{1}H and ^{13}C NMR spectral analysis of (*E*)-asarone and its isomers
L. SIERGIEJCZYK, J. POPLAWSKI, B. LOZOWICKA, A. DUBIS AND B. LACHOWSKA 1037

^{1}H NMR and ^{13}C NMR spectral characterization of some antimalarial *in vitro* 3-amino-9-methyl-1*H*-pyrazolo[3,4-*b*]4-quinolones
J. E. CHARRIS, J. N. DOMÍNGUEZ, G. LOBO, M. I. CORDERO, S. E. LÓPEZ, B. E. MÉNDEZ, S. PEKERAR AND F. RIGGIONE 1039

Conformational analysis of 6-deoxy-6-iodo-D-glucose in aqueous solution
M.-C. BROCHIER-SALON AND C. MORIN 1041

Reassignment of stereochemistry of the 3-ethoxy-2-methyl-2-vinylcyclobutanones
A. SHAGINIAN, M. R. BRENNAN AND K. L. ERICKSON 1043

^{47,49}Ti and ^{13}C NMR spectra of titanium-containing catalysts
A. FORIS **1044**

Book review, 1047; Announcement, 1048; Author index, 1049; Subject index, 1053; Volume contents, i

SPECIAL ISSUE JUNE 2000

Muon Magnetic Resonance
C. J. Rhodes

Guest editorial
C. J. RHODES **S1**

Editorial
H. GÜNTHER **S2**

Muon-spin spectroscopy in selenium
I. D. REID, S. F. J. COX, U. A. JAYASOORIYA AND G. A. HOPKINS **S3**

μSR studies of elemental boron, modelling interstitial protons with implanted positive muons
S. F. J. COX, S. P. COTTRELL, J. S. LORD, C. A. SCOTT, U. A. JAYASOORIYA, G. A. HOPKINS AND N. SULEIMANOV **S9**

Theoretical study on the characterization of the muonium radical in sulfur using ^{33}S hyperfine interactions
B. WEBSTER **S16**

Muonium formation and magnetic relaxation in dextran and iron–dextran
S. H. KILCOYNE AND B. WEBSTER **S20**

Muon radical states in some electron donor and acceptor molecules
F. L. PRATT, S. J. BLUNDELL, TH. JESTÄDT, B. W. LOVETT, R. M. MACRAE AND W. HAYES **S27**

Free radical probes of organic conductor constituents: electronic structures and hyperfine properties
R. M. MACRAE **S33**

Modelling hydrogen transport in molybdenum disulfide catalysts with muon spin relaxation spectroscopy
P. C. H. MITCHELL, D. A. GREEN, E. PAYEN AND C. A. SCOTT **S43**

Hydrogen radioisotopic labelling studies using muonium: properties of thiyl radicals potentially relevant to cellular membrane damage
C. J. RHODES, T. C. DINTINGER, C. S. HINDS, H. MORRIS AND I. D. REID **S49**

Spin-labelling studies of benzene sorbed in carbon particles using muonium: a molecular view of sorption by environmental carbons
C. J. RHODES, T. C. DINTINGER, I. D. REID AND C. A. SCOTT **S58**

Note
Muonium addition to sulfur–nitrogen chains
P. F. KELLY, A. SORIANO-RAMA, P. T. WOOD, I. D. REID, T. A. CLAXTON, C. J. RHODES AND U. A. JAYASOORIYA **S65**

Papers in press, S67